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A

Synopsis

On

"Physicochemical Studies on Metal Complexes of Some Potentially Active Ligands"

For the Degree of

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Under the faculty of Sciences

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Synopsis

Present Work

The work undertaken entitled **"Physicochemical Studies On Metal Complexes of Some Potentially Active Ligands"** includes the synthesis, characterization and biological activities of the ligands and their metal complexes. The work is presented in the thesis in six chapters. A chapter wise summary of the thesis is given below.

Chapter- I

This chapter includes basic concepts of coordination chemistry and its theories in brief. An account of β-diketones, their metal complexes and their importance has been discussed. A brief review of literature on previous studies on diketone complexes related to the present work has been incorporated. At the end of topic the aim of present investigation has also been outlined.

Chapter-II

This chapter includes a) Synthesis of β-diketones and their characterization b) Preparation of transition metal complexes of ligands and their analysis by various physicochemical methods. The six ligands which are prepared are given below.

1. 1-(2-hydroxyphenyl)-3-phenylpropane-1,3-dione.
2. 1-(2-hydroxyphenyl)-3-p-tolylpropane-1,3-dione.
3. 1-(2,4-dichlorophenyl)-3-(2-hydroxyphenyl)propane-1,3-dione.
4. 1-(5-chloro-2-hydroxyphenyl)-3-phenylpropane-1,3-dione.
5. 1-(5-chloro-2-hydroxyphenyl)-3-p-tolylpropane-1,3-dione.
6. 1-(5-chloro-2-hydroxyphenyl)-3-(2,4-dichlorophenyl)propane-1,3-dione.

The general procedure for the preparation of complexes of the ligands, their analysis and characterization by various physicochemical methods is presented.

The same β-diketones and their metal complexes were also synthesized by ultrasound irradiation and characterized.

This chapter also gives the method of elemental analysis for the estimation of metal ions in the complexes followed by analytical data.

Chapter-III

This chapter deals with various experimental techniques employed and their role in the characterization of metal complexes. The experimental details of various techniques used have been given. The techniques used in the present study are magnetic susceptibility measurements, solution conductivity, infrared spectroscopy, ^{1}H-NMR spectroscopy, TGA-DTA, X-ray diffraction.

Chapter-IV

In this chapter the experimental data on conductivity, magnetic susceptibility, electronic absorption spectra and X-ray diffraction measurements of Cu(II), Ni(II), Co(II), Fe(III), Cr(III) complexes are presented and discussed.

Thermal behavior of metal complexes with the help of simultaneous TG-DTA curves has been discussed. Thermodynamic and kinetic parameters for decomposition of metal complexes have been calculated by two different methods. The unit cell data and crystal lattice parameters of metal complexes calculated from strong reflections in the XRD pattern by using computer programming are presented and discussed with respect to Z-values, density, porosity, percentage, crystal system and probable space group.

Chapter-V

This chapter mainly gives results and discussion pertaining to infrared absorption spectra of diketone ligands and their metal complexes. The infrared spectral data are presented and discussed with

respect to assignment of band frequencies for different groups involved in complex formation, mainly from the point of view of locating coordination positions in the metal complexes. The assignments of band frequencies for different groups are empirical and tentative and are based on the information from literature on similar metal complexes.

Chapter-VI

This chapter deals with antibacterial and antifungal activity of ligands and their metal complexes. It is divided into two sections.

Section first includes the experimental procedure for the measurements of antibacterial activity of ligands and their metal complexes tested at concentration of 100ppm solution against Escherichia coli, Bacillus subtilis, Staphylococcus aureus by Kirby Baur's disc diffusion method. The inhibitory zone and data are presented. Antibacterial activity in presence of ligands and metal complexes are studied and compared.

Section second describes introduction to fungi Aspergillus niger and Fusarium oxyporum inparticular. Aspects of fungal growth and their biotechnological, industrial, economic importance and their harmful effects are discussed in brief. The experimental procedure of screening of antifungal activity of ligands and their metal complexes in vitro against Aspergillus niger and Fusarium oxyporum by Kirby Baur's disc diffusion method has been given. The inhibitory zone and data are presented. Fungicidal activities of ligands and metal complexes are compared. It is seen that all the metal complexes show better activity than their parent ligands. At the end of this chapter conclusions drawn from the study are presented.

ORIGINAL WORK

The present work was carried out to understand the structural and biological properties of β-diketones and their metal complexes. These ligands are derived from simple and substituted o-hydroxy acetophenone with different aromatic acids by Baker-Venkatraman transformation and have been used for the first time in the synthesis and studies on structural aspects of Cu(II), Ni(II), Co(II), Fe(III), Cr(III) metal complexes.

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